ELECTRONIC PROPERTIES AND STRUCTURE OF APERIODIC MATERIALS

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Studies, both experimental and theoretical, were made of the electronic properties and structure of aperiodic materials, (amorphous, disordered alloys, surfaces), and of the electronic structure of magnetic materials. By understanding their basic physical mechanisms two old experimental effects were turned into practical tools for measuring fundamental properties of matter. The extended X-ray absorption fine structure can be used to determine the atomic environment around a given type of atom even in complicated aperiodic materials. The magneto-optic Kerr effect can be used to determine the electronic structure of

20. magnetic electrons. Significant contributions were also made to our fundamental knowledge of surfaces and the electronic structure of aperiodic materials.

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Summary of Accomplishments

The research of this final report covers investigations to further our fundamental understanding of aperiodic systems (amorphous, disordered alloys, surfaces, etc.) and the electronic structure of magnetic systems. The significant accomplishments were:

(a) Electronic Properties of Aperiodic Materials.

Showed by optical measurements and theoretical considerations that aperiodic materials can be divided into two classes, A and B. For class A the system can be described by the ideas developed for periodic systems while for class B the disorder is so great that a new theory has to be developed. Significant contributions to developing such a theory were made. Measurements of the variation of the Fermi surface in some class A alloys were made which showed that the classical explanation of the Hume-Rothery rules are incorrect.

(b) Surfaces

The effect of surfaces states on the optical properties of pure metals was shown to be negligible. The second harmonic generation of light at silver surfaces was found to be extremely sensitive to surface contaminants and roughness and a theory was developed to estimate the effect at a clean smooth surface. The work function and surface composition of AgAu alloys were determined for the first time stimulating theoretical interest in the result.

(c) Extended X-ray Absorption Fine Structure (EXAFS).

By understanding the basic physical mechanisms that contribute to the fine structure on the high energy side of the X-ray absorption edges, the EXAFS has been developed into a practical and novel tool to measure the atomic environment around particular types of atoms

in complicated aperiodic materials. The promising potential of EXAFS led to the building of an EXAFS facility at the Stanford Syncrotron radiation source national facility.

(d) Magnetism

By developing further our understanding of the magneto-optic Kerr effect, this effect has now been added to our tools to determine the electronic properties of magnetic materials. It has been used to obtain such information on transition and rare earth metal ferromagnets.

Scientific Personnel - February 1, 1967 to September 30, 1974

A. Faculty E. A. Stern, Professor of Physics

S. C. Fain, Assistant Professor of Physics

J. M. Tracy, Research Associate, 10/1/70 - 9/30/71
(Supported by other funds)

J. L. Erskine, Research Associate 3/16/69 - 6/30/74

Dale E. Sayers, Research Associate 2/16/72 - 9/30/74
(Supported by other funds)

B. Graduate Students

Frank Carman, M.S. (1968).

Graeme Blake, Predoctoral Research Associate
10/1/67 - 9/30/74

Ronald Campbell, Research Associate
10/1/69 - 9/30/71 (supported by other funds)

L. Vincent Corbin, NSF Trainee

James L. Erskine, Research Associate
10/1/69-3/15/72

Christopher Flaten, Predoctoral Research Associate
10/1/67 - 9/5/72

Peter McCardell, Predoctoral Research Associate
10/1/72 - 4/15/73

Dale E. Sayers, Predoctoral Research Associate
10/1/70 - 2/15/72

J. Michael McDavid, Predoctoral Research Associate
10/1/72 - 9/30/74

William B. Vail, Predoctoral Research Associate
10/1/67 - 9/30/74

Avner Zin, Predoctoral Research Associate
12/15/72 - 6/15/73

Bruce Bunker, Undergraduate
6/15/73 - 9/30/74

George T. Cox, Predoctoral Research Associate
9/15/73 - 1/31/74

Haiping Dun, Predoctoral Research Associate
9/15/73 - 6/30/74

Pat Cassidy, Predoctoral Research Associate
12/31/73 - 9/30/74 (supported by other funds)

William Lau, Predoctoral Research Associate
6/30/74 - 9/30/74

Ph.D Degrees Granted

John M. Tracy - "Polar Reflection Faraday Effect in Silver-Based Disordered Alloys" 1970

James L. Erskine - "The Magneto-Optic Kerr Effect in Gadolinium" 1972

Christopher Flaten - "Optical Constants in Silver Alloys" 1972

Dale E. Sayers - "A New Technique to Determine Amorphous Structure Using Extended X-Ray Absorption Fine Structure" 1971

Peter D. McCardell - "The Effect of the Surface on the Generation of Second Harmonic Light by Silver" 1973

Avner Zin - "The Density of States of Disordered Binary Alloys" 1973

William B. Vail - "Fermi Surface Measurements of Disordered Alpha and Beta Phase Ag-Cd Alloys Using the Intraband Polar Reflection Faraday Effect" 1974

Graeme Blake - "Optical Properties of Dy, Tb and Gd" in preparation

Michael McDavid - "Surface Composition and Work Function of Noble Metal Alloys" in preparation

Completed Research

1. "Electron States in Dilute Disordered Alloys," Phys. Rev. 168, 730(1968).

2. "Clean Surface Effects on the Optical Properties of Metals," E. A. Stern, in The Structure and Chemistry of Solid Surfaces, (John Wiley and Sons, N.Y., 1969), Ch. 26.

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4. "Electron Density of States in Dilute Alloys," Phys. Rev. B1, 1518(1970), E. A. Stern.

5. "Point Scattering Theory of X-ray K-Absorption Fine Structure," E. E. Sayers, F. W. Lytle, And E. A. Stern, in Advances in X-Ray Analysis (Plenum Press, 1970), Vol. 13, p. 248.

6. "Conductivity of Magnetic Metals," J. L. Erskine and E. A. Stern, J. Appl. Phys. 41, 1246(1970).

7. "New Technique for Investigating Noncrystalline Structures: Fourier Analysis of the Extended X-Ray Absorption Fine Structure," D. E. Sayers, E. A. Stern and F. W. Lytle, Phys. Rev. Letters 27, 1204(1971).

8. "Structure Determination of Amorphous Ge, GeO_2 and GeSe by Fourier Analysis of Extended X-Ray Absorption Fine Structure (EXAFS)," D. E. Sayers, F. W. Lytle, and E. A. Stern, J. Non. Cryst. Solids 8-10, 401(1972).

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10. "Fermi Level in Disordered Alloys," E. A. Stern, Phys. Rev. B5, 366(1972).

11. "Shielding and Density of States in Alloys," E. A. Stern, Phys. Rev. B7, 5054(1973).

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14. "Electrostatic Deflection Binary Alloy Evaporation," J. L. Erskine, J. M. Tracy and E. A. Stern, Rev. of Sci. Instr. 42, 501(1971).

15. "Magneto-Optic Kerr Effects in Gadolinium Metal," J. Erskine, Ph.D. Thesis.

16. "Magneto-Optic Kerr Effects in Gadolinium," J. L. Erskine and E. A. Stern, Phys. Rev. B 8, 1239(1973).

17. "Optical Constants in Silver Alloys," C. J. Flaten, Ph.D. Thesis. 1972.

18. "Shielding of Impurities as Measured by Extended X-ray Absorption Fine Structure", E. A. Stern and D. Sayers, Phys. Rev. Lett. 30, 174(1973).

19. "Self-Consistent Screening in a Simple Model," J. Rudnick and E. A. Stern, Phys. Rev. B 7, 5062(1973).

20. "Forward Scattering Approximation for Disordered Systems," E. A. Stern, Phys. Rev. B 7, 1303(1973).

21. "Polar Reflection Faraday Effect in α-Phase Disordered Alloy of Silver," John Tracy and E. A. Stern, Phys. Rev. B 8, 582(1973).

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23. "Faraday Rotation and the Electronic Structure of Alloys," (Phila.), Chapter in book, Charge Transfer/Electronic Structure of Alloys, (AIME Publishers, N. Y., 1974) edited by R. H. Bennett and R. H. Willens, p. 197.

24. "Determination of Local Structure in Amorphous GeSe, $GeSe_2$, As_2Se_3, As_2S_3 and As_2Te_3 Using EXAFS," D. E. Sayers, F. Lytle and E. A. Stern. Talk given at 5th International Conference on Amorphous and Liquid Semiconductors Sept. 1973. (Garmisch-Partenkirchen, West Germany). Amorphous and Liquid Semiconductors (Taylor and Francis Ltd., London, 1974) edited by J. Stuke and W. Brenig, pp. 403-412.

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27. "The Density of States of Disordered Binary Alloys," Avner Zin, Ph.D. Thesis. (1973).

28. "Work Function of Silver-Gold Alloys," S. C. Fain, Jr. and J. M. McDavid, Bull. Am. Phys. Soc. 18, 425(1973).

29. "Surface Composition and Work Function of Silver-Gold Alloys," S. C. Fain, Jr. and J. M. McDavid, Abstracts from Thirty-Third Annual Conference on Physical Electronics, University of Calif., Berkeley (26-28 March 1973), p. 6.

30. "The Effect of the Surface on the Generation of Second Harmonic Light by Silver," Peter McCardell, Ph.D. Thesis. (1973)

31. "Application of Alloy Physics to Solution Hardening," Invited talk given at Oct. 1973 meeting of ASM (Chicago). To be published as chapter in book.

32. "Theory of Extended X-ray Absorption Fine Structure, E. A. Stern Phys. Rev. to be published in Phys. Rev. B, Sept. 15, 1974.

33. "Fermi Surface Measurements of Disordered Alpha and Beta Phase Ag-Cd Alloys Using the Intraband Polar Reflection Faraday Effect," W. B. Vail, III, Ph.D. Thesis. (1974).

34. "Optical Properties of Gd, Dy, and Tb," J. L. Erskine, G. A. Blake and C. J. Flaten, Journal of the Optical Society of America, 64, 1332(1974).

35. "Work-function Variation with Alloy Composition: Ag-Au," S. C. Fain, Jr. and J. M. McDavid, Phys. Rev. B 9, 5099(1974).

36. "Generalized Coherent-Potential Method for Disordered Systems," E. A. Stern and Avner Zin, Phys. Rev. B 9, 1170(1974).

37. "Second Harmonic Radiation from a Metal Surface," J. Rudnick and E. A. Stern, Proceedings of Sicily Conference on Excitations in Solids, Summer 1973.

38. "Optical Constants of Some Silver Alloys, C. Flaten, E. A. Stern, Phys. Rev., (accepted for publication).

39. "Segregation at Cu-Au Alloy Surfaces," J. M. McDavid and S. C. Fain, Jr. (in preparation).

40. "The Density of States of Disordered Binary Alloys," Avner Zin and E. A. Stern (in preparation).

41. "The Effect of the Surface on the Generation of Second Harmonic Light by Silver," P. McCardell and E. A. Stern (in preparation).

42. "Fermi Surface Measurements of Disordered Alpha and Beta Phase Ag-Cd Alloys Using the Intraband Polar Reflection Faraday Effect," W. B. Vail and E. A. Stern (in preparation).

COUPLING

1. Electronic Structure of Disordered Solids DATE: 1969-70

   a. E. A. Stern, Professor of Physics
   b. Research Association with BSRL
   c. Our research group has very close contact with the Boeing Scientific Research Laboratory. Our of my students, Mr. Dale Sayers, is doing a research project on amorphous solids using the research facilities at B.S.R.L. Related to this project and because of our common interest in this problem, I have had frequent contacts with Mr. Farrell Lytle and Dr. Hans Brunner, head of B.S.R.L.'s Solid State Division. In addition I have had several conversations with Dr. Allan Smith of B.S.R.L. concerning our common interest in surfaces.

2. Extended x-ray absorption fine structure (EXAFS) DATE: 1968-1974

   a. E. A. Stern, Professor of Physics
   b. Consultant to Boeing Company
   c. Professor Stern has been consulting with the Boeing Company in regard to EXAFS. The research results on EXAFS are a joint effort with Dr. Dale Sayers and Mr. Farrel Lytle, both of the Boeing Company.

3. Auger spectroscopy of thin alloy films DATE: 6/1/72 - 9/30/72

   a. Professor S. C. Fain, Jr.,
   b. Collaboration with Washington State University (WSU)
   c. Auger spectroscopy measurements on alloy thin film samples prepared at University of Washington have been carried out at WSU. These measurements demonstrated the feasibility of research proposed by WSU to DOD agencies.

4. Work function and surface composition of alloys DATE: 1973

   a. Professor S. C. Fain, Jr.
   b. Seminar and discussion
   c. A seminar summarizing the existing information on work function of alloys was presented at General Motors Research Laboratories. A discussion was held with Dr. Frank Williams regarding predictions of his theory for surface composition of alloys. Also, the problem of nitriding of steels was discussed with Dr. Gary Tivetts.

5. Application of Alloy Physics to Solution Hardening

   a. Professor E. A. Stern, University of Washington
   b. Invited talk at Materials Science Congress, October 1973
   c. Professor Stern was invited to speak at a session chaired by Drs. H. Gegel and E. Collings. He also spent some time discussing this and related topics with the chairmen. Dr. H. Gegel is permanently located at the Air Force Materials Laboratory, Wright-Patterson Air Force Base, Ohio.

6. Faraday Rotation and the Electronic Structure of Alloys

   a. Professor E. A. Stern, University of Washington
   b. Invited talk at the Metallurgical Society-AIME annual Spring meeting May 1973.
   c. Professor Stern was invited to speak at a session on the Electronic Structure of Alloys. Among the participants speaking was one from McDonnell-Douglass. The topic of the session was pertinent to areas of interest to the Air Force.

7. Requirements for a Calculation of Phase Equilibrium of Disordered Alloys.

   a. Professor E. A. Stern, University of Washington
   b. Invited talk at the American Society of Metals - 1974 Materials Science Symposium, Oct. 23, 1974.
   c. The session which included Professor Stern's talk was devoted to Methods for Estimating the Stability of Metallic Phases; a topic pertinent to Air Force interests.